

Author index to volume 196

Abbate, F., see Marconi, G.	196 (1995) 383
Adamowicz, L., see Gutsev, G.L.	196 (1995) 1
Ågren, H., O. Vahtras and V. Carravetta, Near-edge core photoabsorption in polyacenes:	
model molecules for graphite	196 (1995) 47
Alekseyev, A.B., see Das, K.K.	196 (1995) 395
Allnatt, A.R., see Dham, A.K.	196 (1995) 81
Alon, O.E. and N. Moiseyev, Broken dynamical symmetry condition to control a chemical	
reaction by the complex coordinate (t, t') method	196 (1995) 499
Alonso, J.A., see Glossman, M.D.	196 (1995) 455
Angeloni, L., see Marconi, G.	196 (1995) 383
Azinović, D., S. Milošević and G. Pichler, Photochemical population of KHg* states	196 (1995) 267
Bagryansky, V.A., see Korolev, V.V.	196 (1995) 317
Balbás, L.C., see Glossman, M.D.	196 (1995) 455
Baltzer, P., B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A. MacDonald and W. von Niessen, An experimental and theoretical study of the valence shell	
photoelectron spectrum of allene	196 (1995) 551
Bartocci, G., see Marconi, G.	196 (1995) 383
Bazhin, N.M., see Korolev, V.V.	196 (1995) 317
Becker, S., C. Braatz, J. Lindner and E. Tiemann, Investigation of the predissociation of	
SO ₂ : state selective detection of the SO and O fragments	196 (1995) 275
Besnard, M., see Zoidis, E.	196 (1995) 521
Bettermann, H. and I. Dasting, Excited-state geometries derived from the analysis of	
resonance Raman spectra. Example: $(\pi - \pi^*)$ state of 3,5-di-tert-butyl-o-benzoquinone	196 (1995) 531
Bolotsky, V.V., see Korolev, V.V.	196 (1995) 317
Braatz, C., see Becker, S.	196 (1995) 275
Brion, C.E., see Cooper, G.	196 (1995) 293
Brion, C.E., see Hollebone, B.P.	196 (1995) 13
Broo, A. and M.C. Zerner, Electronic structure of donor-spacer-acceptor molecules of	
potential interest for molecular electronics. III. Geometry and absorption spectrum of CH ₃ -α P3CNQ	196 (1995) 407
Broo, A. and M.C. Zerner, Electronic structure of donor-spacer-acceptor molecules of potential interest for molecular electronics. IV. Geometry and device properties of	270 (2770) 101
P3CNQ and Q3CNQ	196 (1995) 423
Buenker, R.J., see Das, K.K.	196 (1995) 395
Buonomo, E. and F.A. Gianturco, Metastable decay of ionic argon clusters: rotational	170 (1775) 375
predissociation of (Ar) ₄ ⁺	196 (1995) 465
Burton, G.R., see Cooper, G.	196 (1995) 293
1	



Author index to volume 196

Abbate, F., see Marconi, G.	196 (1995) 383
Adamowicz, L., see Gutsev, G.L.	196 (1995) 1
Ågren, H., O. Vahtras and V. Carravetta, Near-edge core photoabsorption in polyacenes:	
model molecules for graphite	196 (1995) 47
Alekseyev, A.B., see Das, K.K.	196 (1995) 395
Allnatt, A.R., see Dham, A.K.	196 (1995) 81
Alon, O.E. and N. Moiseyev, Broken dynamical symmetry condition to control a chemical	
reaction by the complex coordinate (t, t') method	196 (1995) 499
Alonso, J.A., see Glossman, M.D.	196 (1995) 455
Angeloni, L., see Marconi, G.	196 (1995) 383
Azinović, D., S. Milošević and G. Pichler, Photochemical population of KHg* states	196 (1995) 267
Bagryansky, V.A., see Korolev, V.V.	196 (1995) 317
Balbás, L.C., see Glossman, M.D.	196 (1995) 455
Baltzer, P., B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A. MacDonald and W. von Niessen, An experimental and theoretical study of the valence shell	
photoelectron spectrum of allene	196 (1995) 551
Bartocci, G., see Marconi, G.	196 (1995) 383
Bazhin, N.M., see Korolev, V.V.	196 (1995) 317
Becker, S., C. Braatz, J. Lindner and E. Tiemann, Investigation of the predissociation of	
SO ₂ : state selective detection of the SO and O fragments	196 (1995) 275
Besnard, M., see Zoidis, E.	196 (1995) 521
Bettermann, H. and I. Dasting, Excited-state geometries derived from the analysis of	
resonance Raman spectra. Example: $(\pi - \pi^*)$ state of 3,5-di-tert-butyl-o-benzoquinone	196 (1995) 531
Bolotsky, V.V., see Korolev, V.V.	196 (1995) 317
Braatz, C., see Becker, S.	196 (1995) 275
Brion, C.E., see Cooper, G.	196 (1995) 293
Brion, C.E., see Hollebone, B.P.	196 (1995) 13
Broo, A. and M.C. Zerner, Electronic structure of donor-spacer-acceptor molecules of	
potential interest for molecular electronics. III. Geometry and absorption spectrum of CH ₃ -α P3CNQ	196 (1995) 407
Broo, A. and M.C. Zerner, Electronic structure of donor-spacer-acceptor molecules of potential interest for molecular electronics. IV. Geometry and device properties of	270 (2770) 101
P3CNQ and Q3CNQ	196 (1995) 423
Buenker, R.J., see Das, K.K.	196 (1995) 395
Buonomo, E. and F.A. Gianturco, Metastable decay of ionic argon clusters: rotational	170 (1775) 375
predissociation of (Ar) ₄ ⁺	196 (1995) 465
Burton, G.R., see Cooper, G.	196 (1995) 293
1	

Carravetta, V., see Ågren, H.	196 (1995) 47
Castellucci, E., see Marconi, G.	196 (1995) 383
Chan, W.F., see Cooper, G.	196 (1995) 293
Cooper, G., G.R. Burton, W.F. Chan and C.E. Brion, Absolute oscillator strengths for the	
photoabsorption of silane in the valence and Si 2p and 2s regions (7.5-350 eV)	196 (1995) 293
Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Pseudopotential calculations for the	
potential energies of LiHe and BaHe	196 (1995) 37
Dähne, L., A. Horvath and G. Weiser, Influence of aggregation on the optical spectra of a	
polymethine dye in single crystals	196 (1995) 307
Das, K.K., A.B. Alekseyev, HP. Liebermann, G. Hirsch and R.J. Buenker, Spin-orbit	(,
configuration interaction study of the electronic spectrum of antimony iodide	196 (1995) 395
Dasting, I., see Bettermann, H.	196 (1995) 531
Davidson, E.R., see Hollebone, B.P.	196 (1995) 13
Dham, A.K. and W.J. Meath, Exchange-Coulomb potential energy surfaces, and related	
physical properties, for Kr-N ₂	196 (1995) 125
Dham, A.K., A.R. Allnatt, A. Koide and W.J. Meath, Representations of dispersion energy	
damping functions for interactions of closed shell atoms and molecules	196 (1995) 81
Dibble, T.S., see Su, Y.	196 (1995) 59
Dmitryuk, A.V., see Syutkin, V.M.	196 (1995) 139
Dorfmüller, T., see Zoidis, E.	196 (1995) 171
Dupré, P., P.G. Green and R.W. Field, Quantum beat spectroscopic studies of Zeeman	
anticrossings in the \tilde{A}^1A_u state of the acetylene molecule (C_2H_2)	196 (1995) 211
Dupré, P., Study of Zeeman anticrossing spectra of the AlAu state of the acetylene	
molecule (C_2H_2) by Fourier transform: product $\rho_{vib}\langle V\rangle$ and isomerization barrier	196 (1995) 239
Dyke, J.M., see Haggerston, D.	196 (1995) 353
Ferretti, A., A. Lami and G. Villani, Control of the yield of photophysical/photochemical	
processes by excitation with properly delayed ultrashort phase-locked light pulses: a	
model study on the pyrazine $S_2 \rightarrow S_1$ internal conversion	196 (1995) 447
Field, R.W., see Dupré, P.	196 (1995) 211
Fischer, G., see Nicholson, J.A.	196 (1995) 327
Francisco, J.S., see Su, Y.	196 (1995) 59
Fujimura, Y., see Sugawara, M.	196 (1995) 113
Fuß, W., K.L. Kompa and S. Weizbauer, IR spectrum of HCF2CF2Br: hindered intramolec-	
ular vibrational energy redistribution	196 (1995) 179
Gianturco, F.A. and S. Kumar, Dynamics of vibrationally inelastic collisions in H ⁺ -H ₂ :	
comparing quantum calculations with experiments	196 (1995) 485
Gianturco, F.A., see Buonomo, E.	196 (1995) 465
Glossman, M.D., L.C. Balbás and J.A. Alonso, Incipient manifestation of the shell structure	
of atoms within the WDA model for the exchange and kinetic energy density functionals	196 (1995) 455
Green, P.G., see Dupré, P.	196 (1995) 211
Gutsev, G.L., A.L. Sobolewski and L. Adamowicz, A theoretical study on the structure of	
acetonitrile (CH ₃ CN) and its anion CH ₃ CN ⁻	196 (1995) 1

Haggerston, D., J.M. Dyke and A. Morris, The use of UV photoelectron spectroscopy to	
monitor production of excited states of atomic lead from the $Pb(^{3}P_{0}) + O_{2}(a^{1}\Delta_{g})$	
reaction	196 (1995) 353
Hirsch, G., see Das, K.K.	196 (1995) 395
Holland, D.M.P., see Baltzer, P.	196 (1995) 551
Hollebone, B.P., J.J. Neville, Y. Zheng, C.E. Brion, Y. Wang and E.R. Davidson, Valence	
electron momentum distributions of ethylene; comparison of EMS measurements with	
near Hartree-Fock limit, configuration interaction and density functional theory calcula-	
tions	196 (1995) 13
Horvath, A., see Dähne, L.	196 (1995) 307
Huizer, A.H., see van der Burgt, M.J.	196 (1995) 193
Im, HS., see Kang, W.K.	196 (1995) 363
Jung, KH., see Kang, W.K.	196 (1995) 363
Jung, K.W., see Kang, W.K.	196 (1995) 363
6,	
Kang, W.K., K.W. Jung, D.C. Kim, KH. Jung and HS. Im, Energy partitioning in	
photodissociation of methyl, ethyl and <i>n</i> -propyl iodides at 304 nm	196 (1995) 363
Kapsomenos, G., see Karafiloglou, P.	196 (1995) 69
Karafiloglou, P. and G. Kapsomenos, Local description of a polyenic radical cation	196 (1995) 69
Karlsson, L., see Baltzer, P.	196 (1995) 551
Kim, D.C., see Kang, W.K.	196 (1995) 363
Koide, A., see Dham, A.K.	196 (1995) 81
Kompa, K.L., see Fuß, W.	196 (1995) 179
Korolev, V.V., V.V. Bolotsky, N.V. Shokhirev, E.B. Krissinel', V.A. Bagryansky and	170 (1775) 177
N.M. Bazhin, Diffusion of molecular oxygen in glassy matrices, studied by lumines-	
cence quenching	196 (1995) 317
Krissinel', E.B., see Korolev, V.V.	196 (1995) 317
Kumar, S., see Gianturco, F.A.	196 (1995) 485
Rullat, 5., see Glantateo, 1.74.	170 (1775) 405
Lami, A., see Ferretti, A.	196 (1995) 447
Lawrance, W.D., see Nicholson, J.A.	196 (1995) 327
Li, Z., see Su, Y.	196 (1995) 59
Liebermann, HP., see Das, K.K.	196 (1995) 395
Lindner, J., see Becker, S.	196 (1995) 275
Luna, A., M. Merchán and B.O. Roos, A theoretical analysis of the lowest excited states in	190 (1993) 213
HNO/NOH and HPO/POH	196 (1995) 437
Lundqvist, M., see Baltzer, P.	196 (1995) 551
	196 (1995) 193
Lusztyk, J., see van der Burgt, M.J.	190 (1993) 193
MacDonald, M.A., see Baltzer, P.	196 (1995) 551
Marconi, G., G. Bartocci, U. Mazzucato, A. Spalletti, F. Abbate, L. Angeloni and E.	170 (1775) 551
Castellucci, Role of internal conversion on the excited state properties of trans-styryl-	
pyridines	196 (1995) 383
Martin, JP., see Wallaart, H.L.	196 (1995) 149
Mazzucato, U., see Marconi, G.	196 (1995) 383
randomy, or, our random, or	170 (1775) 303

Meath, W.J., see Dham, A.K.	196 (1995) 125
Meath, W.J., see Dham, A.K.	196 (1995) 81
Merchán, M., see Luna, A.	196 (1995) 437
Miller, T.A., see Preppernau, B.L.	196 (1995) 371
Milošević, S., see Azinović, D.	196 (1995) 267
Moiseyev, N., see Alon, O.E.	196 (1995) 499
Morris, A., see Haggerston, D.	196 (1995) 353
North, Til, Get Mage-Mon, 21	170 (1775) 555
Neville, J.J., see Hollebone, B.P.	196 (1995) 13
Nicholson, J.A., W.D. Lawrance and G. Fischer, Single vibronic level fluorescence spectra	
from \tilde{A} ($^{1}B_{2u}$) benzene: Fermi resonances and S_{0} IVR lifetimes	196 (1995) 327
Otorbaev, D.K., Catalytic properties of surfaces with respect to generation of CO ₂	
molecules in the plasma	196 (1995) 543
	270 (2770) 0 10
Panich, A.M., NMR study of the F-H · · · F hydrogen bond. Relation between hydrogen	
atom position and F-H · · · F bond length	196 (1995) 511
Paramzina, S.E., see Syutkin, V.M.	196 (1995) 139
Pearce, K., see Preppernau, B.L.	196 (1995) 371
Perrin, MY., see Wallaart, H.L.	196 (1995) 149
Piar, B., see Wallaart, H.L.	196 (1995) 149
Pichler, G., see Azinović, D.	196 (1995) 267
Preppernau, B.L., K. Pearce, A. Tserepi, E. Wurzberg and T.A. Miller, Angular momentum	
state mixing and quenching of $n = 3$ atomic hydrogen fluorescence	196 (1995) 371
Preuss, H., see Czuchaj, E.	196 (1995) 37
Rebentrost, F., see Czuchaj, E.	196 (1995) 37
Roos, B.O., see Luna, A.	196 (1995) 437
	() !
Savel'ev, V.A., see Sokolov, N.D.	196 (1995) 583
Shokhirev, N.V., see Korolev, V.V.	(
bildinine, 11, 11, 500 Itolote, 11, 11	196 (1995) 317
Sobolewski, A.L., see Gutsev, G.L.	196 (1995) 317 196 (1995) 1
Sobolewski, A.L., see Gutsev, G.L.	
Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for	
Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics	196 (1995) 1
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. 	196 (1995) 1 196 (1995) 583
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. 	196 (1995) 1 196 (1995) 583 196 (1995) 383
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 37
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study Sugawara, M. and Y. Fujimura, Control of quantum dynamics by a locally optimized laser 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 37 196 (1995) 59
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study Sugawara, M. and Y. Fujimura, Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation of hydrogen fluoride 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 37
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study Sugawara, M. and Y. Fujimura, Control of quantum dynamics by a locally optimized laser 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 37 196 (1995) 59
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study Sugawara, M. and Y. Fujimura, Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation of hydrogen fluoride Syutkin, V.M., V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina, Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na₂O-12.8CaO-50P₂O₅ 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 37 196 (1995) 59 196 (1995) 113 196 (1995) 139
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study Sugawara, M. and Y. Fujimura, Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation of hydrogen fluoride Syutkin, V.M., V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina, Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na₂O-12.8CaO-50P₂O₅ Tiemann, E., see Becker, S. 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 59 196 (1995) 113 196 (1995) 139 196 (1995) 275
 Sobolewski, A.L., see Gutsev, G.L. Sokolov, N.D. and V.A. Savel'ev, Isotope effects in weak hydrogen bonds. Allowance for two stretching and two bending modes of the A-HB fragment (Chemical Physics 181 (1994) 305-317) Spalletti, A., see Marconi, G. Springborg, M., On electron localization in periodic (C₂H_nCl_{4-n})_x polymers Stoll, H., see Czuchaj, E. Su, Y., T.S. Dibble, J.S. Francisco and Z. Li, Dissociation of acetyl bromide: an experimental and theoretical study Sugawara, M. and Y. Fujimura, Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation of hydrogen fluoride Syutkin, V.M., V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina, Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na₂O-12.8CaO-50P₂O₅ 	196 (1995) 1 196 (1995) 583 196 (1995) 383 196 (1995) 101 196 (1995) 37 196 (1995) 59 196 (1995) 113 196 (1995) 139

	(
Vahtras, O., see Ågren, H.	196 (1995) 47
van der Burgt, M.J., A.H. Huizer, C.A.G.O. Varma, B.D. Wagner and J. Lusztyk, Evidence	
for molecular distortion involving the carbonyl group in triplet states of carbonyl	
derivatives of naphthalene obtained from time resolved vibrational spectroscopic studies	196 (1995) 193
Varma, C.A.G.O., see van der Burgt, M.J.	196 (1995) 193
Vauthey, E., Isomerisation dynamics of a thiacarbocyanine dye in different electronic states	
and in different classes of solvents	196 (1995) 569
Villani, G., see Ferretti, A.	196 (1995) 447
von Niessen, W., see Baltzer, P.	196 (1995) 551
Wagner, B.D., see van der Burgt, M.J.	196 (1995) 193
Wallaart, H.L., B. Piar, MY. Perrin and JP. Martin, Transfer of vibrational energy to	
electronic excited states and vibration enhanced carbon production in optically excited	
V-V pumped CO	196 (1995) 149
Wang, Y., see Hollebone, B.P.	196 (1995) 13
Wannberg, B., see Baltzer, P.	196 (1995) 551
Weiser, G., see Dähne, L.	196 (1995) 307
Weizbauer, S., see Fuß, W.	196 (1995) 179
Wurzberg, E., see Preppernau, B.L.	196 (1995) 371
Yarwood, J., see Zoidis, E.	196 (1995) 521
Zerner, M.C., see Broo, A.	196 (1995) 407
Zerner, M.C., see Broo, A.	196 (1995) 423
Zheng, Y., see Hollebone, B.P.	196 (1995) 13
Zoidis, E. and T. Dorfmüller, Far infrared interaction induced absorption spectra of	
CS ₂ -C ₆ H ₆ liquid mixtures. A low concentration study	196 (1995) 171
Zoidis, E., M. Besnard and J. Yarwood, An infrared study of the interaction-induced	
vibrational spectra of benzene in liquid binary mixtures containing CS ₂ and C ₆ F ₆	196 (1995) 521

Subject index to volume 196

Methods

Theoretical

Many body and quasiparticle approaches	
A theoretical study on the structure of acetonitrile (CH ₃ CN) and its anion CH ₃ CN ⁻ , G.L.	10((1005) 1
Gutsev, A.L. Sobolewski and L. Adamowicz	196 (1995) 1
Valence electron momentum distributions of ethylene; comparison of EMS measurements with near Hartree-Fock limit, configuration interaction and density functional theory calculations, B.P. Hollebone, J.J. Neville, Y. Zheng, C.E. Brion, Y. Wang and E.R. Davidson	196 (1995) 13
Relativistic quantum mechanics	
Spin-orbit configuration interaction study of the electronic spectrum of antimony iodide,	
K.K. Das, A.B. Alekseyev, HP. Liebermann, G. Hirsch and R.J. Buenker	196 (1995) 395
Ab initio schemes for stationary properties	
A theoretical study on the structure of acetonitrile (CH ₃ CN) and its anion CH ₃ CN ⁻ , G.L.	
Gutsev, A.L. Sobolewski and L. Adamowicz	196 (1995) 1
Pseudopotential calculations for the potential energies of LiHe and BaHe, E. Czuchaj, F.	
Rebentrost, H. Stoll and H. Preuss	196 (1995) 37
Near-edge core photoabsorption in polyacenes: model molecules for graphite, H. Ågren, O.	
Vahtras and V. Carravetta	196 (1995) 47
Dissociation of acetyl bromide: an experimental and theoretical study, Y. Su, T.S. Dibble,	
J.S. Francisco and Z. Li	196 (1995) 59
Local description of a polyenic radical cation, P. Karafiloglou and G. Kapsomenos	196 (1995) 69
Representations of dispersion energy damping functions for interactions of closed shell	
atoms and molecules, A.K. Dham, A.R. Allnatt, A. Koide and W.J. Meath	196 (1995) 81
On electron localization in periodic $(C_2H_nCl_{4-n})_x$ polymers, M. Springborg	196 (1995) 101
Spin-orbit configuration interaction study of the electronic spectrum of antimony iodide,	
K.K. Das, A.B. Alekseyev, HP. Liebermann, G. Hirsch and R.J. Buenker	196 (1995) 395
Electronic structure of donor–spacer–acceptor molecules of potential interest for molecular electronics. III. Geometry and absorption spectrum of CH ₃ -α P3CNQ, A. Broo and M.C.	
Zerner	196 (1995) 407

A theoretical analysis of the lowest excited states in HNO/NOH and HPO/POH, A. Luna, M. Merchán and B.O. Roos	196 (1995) 437
Computational and simulation methods	
Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation	104 (1005) 115
of hydrogen fluoride, M. Sugawara and Y. Fujimura Exchange—Coulomb potential energy surfaces, and related physical properties, for Kr-N ₂ ,	196 (1995) 113
A.K. Dham and W.J. Meath	196 (1995) 125
Electronic structure of donor–spacer–acceptor molecules of potential interest for molecular electronics. III. Geometry and absorption spectrum of CH ₃ -α P3CNQ, A. Broo and M.C.	105 (1005) 105
Zerner Electronic structure of donor–spacer–acceptor molecules of potential interest for molecular	196 (1995) 407
electronics. IV. Geometry and device properties of P3CNQ and Q3CNQ, A. Broo and M.C. Zerner	196 (1995) 423
Control of the yield of photophysical/photochemical processes by excitation with properly	()
delayed ultrashort phase-locked light pulses: a model study on the pyrazine $S_2 \rightarrow S_1$	107 (1005) 447
internal conversion, A. Ferretti, A. Lami and G. Villani Incipient manifestation of the shell structure of atoms within the WDA model for the	196 (1995) 447
exchange and kinetic energy density functionals, M.D. Glossman, L.C. Balbás and J.A.	
Alonso	196 (1995) 455
Molecular dynamics and scattering theory	
Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation	(
of hydrogen fluoride, M. Sugawara and Y. Fujimura Control of the yield of photophysical/photochemical processes by excitation with properly	196 (1995) 113
delayed ultrashort phase-locked light pulses: a model study on the pyrazine $S_2 \rightarrow S_1$	
internal conversion, A. Ferretti, A. Lami and G. Villani	196 (1995) 447
Metastable decay of ionic argon clusters: rotational predissociation of (Ar) ₄ ⁺ , E. Buonomo and F.A. Gianturco	196 (1995) 465
Dynamics of vibrationally inelastic collisions in H^+-H_2 : comparing quantum calculations	190 (1993) 403
with experiments, F.A. Gianturco and S. Kumar	196 (1995) 485
Broken dynamical symmetry condition to control a chemical reaction by the complex coordinate (t, t') method, O.E. Alon and N. Moiseyev	106 (1005) 400
coordinate (t, t) method, O.E. Alon and N. Moiseyev	196 (1995) 499
Experimental	
Magnetic resonances	
Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na ₂ O-12.8CaO-	
50P ₂ O ₅ , V.M. Syutkin, V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina NMR study of the F-H···F hydrogen bond. Relation between hydrogen atom position	196 (1995) 139
and F-H · · · F bond length, A.M. Panich	196 (1995) 511
Infrared spectroscopy	
Transfer of vibrational energy to electronic excited states and vibration enhanced carbon production in optically excited V-V pumped CO, H.L. Wallaart, B. Piar, MY. Perrin and JP. Martin	196 (1995) 149
and J1. Martin	190 (1993) 149

Far infrared interaction induced absorption spectra of CS ₂ -C ₆ H ₆ liquid mixtures. A low concentration study, E. Zoidis and T. Dorfmüller	196 (1995) 171
IR spectrum of HCF ₂ CF ₂ Br: hindered intramolecular vibrational energy redistribution, W.	190 (1993) 171
Fuß, K.L. Kompa and S. Weizbauer	196 (1995) 179
An infrared study of the interaction-induced vibrational spectra of benzene in liquid binary mixtures containing CS_2 and $\mathrm{C}_6\mathrm{F}_6$, E. Zoidis, M. Besnard and J. Yarwood	196 (1995) 521
Raman spectroscopy Evidence for molecular distortion involving the carbonyl group in triplet states of carbonyl derivatives of naphthalene obtained from time resolved vibrational spectroscopic studies, M.J. van der Burgt, A.H. Huizer, C.A.G.O. Varma, B.D. Wagner and J. Lusztyk	196 (1995) 193
Excited-state geometries derived from the analysis of resonance Raman spectra. Example:	196 (1993) 193
$^{1}(\pi-\pi^{*})$ state of 3,5-di-tert-butyl-o-benzoquinone, H. Bettermann and I. Dasting	196 (1995) 531
Visible and UV spectroscopy	
Transfer of vibrational energy to electronic excited states and vibration enhanced carbon production in optically excited V-V pumped CO, H.L. Wallaart, B. Piar, MY. Perrin	
and JP. Martin	196 (1995) 149
Study of Zeeman anticrossing spectra of the \tilde{A}^1A_u state of the acetylene molecule (C_2H_2) by Fourier transform: product $\rho_{vib}\langle V \rangle$ and isomerization barrier, P. Dupré	196 (1995) 239
Photochemical population of KHg* states, D. Azinović, S. Milošević and G. Pichler	196 (1995) 267
Investigation of the predissociation of SO ₂ : state selective detection of the SO and O	
fragments, S. Becker, C. Braatz, J. Lindner and E. Tiemann	196 (1995) 275
Absolute oscillator strengths for the photoabsorption of silane in the valence and Si 2p and 2s regions (7.5–350 eV), G. Cooper, G.R. Burton, W.F. Chan and C.E. Brion	196 (1995) 293
Influence of aggregation on the optical spectra of a polymethine dye in single crystals, L.	
Dähne, A. Horvath and G. Weiser	196 (1995) 307
A theoretical analysis of the lowest excited states in HNO/NOH and HPO/POH, A. Luna, M. Merchán and B.O. Roos	196 (1995) 437
Catalytic properties of surfaces with respect to generation of CO ₂ molecules in the plasma,	()
D.K. Otorbaev	196 (1995) 543
Fluorescence spectroscopy	
Diffusion of molecular oxygen in glassy matrices, studied by luminescence quenching,	
V.V. Korolev, V.V. Bolotsky, N.V. Shokhirev, E.B. Krissinel', V.A. Bagryansky and N.M. Bazhin	196 (1995) 317
Single vibronic level fluorescence spectra from \tilde{A} ($^{1}B_{2u}$) benzene: Fermi resonances and S_0	190 (1993) 317
IVR lifetimes, J.A. Nicholson, W.D. Lawrance and G. Fischer	196 (1995) 327
Photoelectron and Auger spectroscopy	
The use of UV photoelectron spectroscopy to monitor production of excited states of	
atomic lead from the Pb(3P_0) + O ₂ (a $^1\Delta_g$) reaction, D. Haggerston, J.M. Dyke and A. Morris	196 (1995) 353
An experimental and theoretical study of the valence shell photoelectron spectrum of	190 (1993) 333
allene, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A.	
MacDonald and W. von Niessen	196 (1995) 551

X-ray spectroscopy	
Near-edge core photoabsorption in polyacenes: model molecules for graphite, H. Ågren, O. Vahtras and V. Carravetta	196 (1995) 47
Electron impact spectroscopy	
Valence electron momentum distributions of ethylene; comparison of EMS measurements with near Hartree-Fock limit, configuration interaction and density functional theory calculations, B.P. Hollebone, J.J. Neville, Y. Zheng, C.E. Brion, Y. Wang and E.R. Davidson	196 (1995) 13
Davidson	150 (1555) 15
Laser methods	
Dissociation of acetyl bromide: an experimental and theoretical study, Y. Su, T.S. Dibble,	104 (1005) 50
J.S. Francisco and Z. Li	196 (1995) 59
Photochemical population of KHg* states, D. Azinović, S. Milošević and G. Pichler Investigation of the predissociation of SO ₂ : state selective detection of the SO and O	196 (1995) 267
fragments, S. Becker, C. Braatz, J. Lindner and E. Tiemann	196 (1995) 275
Angular momentum state mixing and quenching of $n = 3$ atomic hydrogen fluorescence,	190 (1993) 213
B.L. Preppernau, K. Pearce, A. Tserepi, E. Wurzberg and T.A. Miller	196 (1995) 371
Picosecond spectroscopy	
Role of internal conversion on the excited state properties of trans-styrylpyridines, G.	
Marconi, G. Bartocci, U. Mazzucato, A. Spalletti, F. Abbate, L. Angeloni and E.	10 ((100 %) 400
Castellucci	196 (1995) 383
Isomerisation dynamics of a thiacarbocyanine dye in different electronic states and in different classes of solvents, E. Vauthey	196 (1995) 569
Non-linear optical spectroscopy	
Angular momentum state mixing and quenching of $n = 3$ atomic hydrogen fluorescence, B.L. Preppernau, K. Pearce, A. Tserepi, E. Wurzberg and T.A. Miller	196 (1995) 371
Synchrotron spectroscopies	
Near-edge core photoabsorption in polyacenes: model molecules for graphite, H. Ågren, O. Vahtras and V. Carravetta	196 (1995) 47
An experimental and theoretical study of the valence shell photoelectron spectrum of allene, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A.	
MacDonald and W. von Niessen	196 (1995) 551
Atomic and molecular beam techniques	
A theoretical study on the structure of acetonitrile (CH ₃ CN) and its anion CH ₃ CN ⁻ , G.L. Gutsev, A.L. Sobolewski and L. Adamowicz	196 (1995) 1
Energy partitioning in photodissociation of methyl, ethyl and <i>n</i> -propyl iodides at 304 nm,	170 (1773) 1
W.K. Kang, K.W. Jung, D.C. Kim, KH. Jung and HS. Im	196 (1995) 363
Time-resolved experiments	
Evidence for molecular distortion involving the carbonyl group in triplet states of carbonyl	
derivatives of naphthalene obtained from time resolved vibrational spectroscopic studies,	
M.J. van der Burgt, A.H. Huizer, C.A.G.O. Varma, B.D. Wagner and J. Lusztyk	196 (1995) 193
Taglet and J. Misztyk	170 (1775) 13

196 (1995) 307

Quantum beat spectroscopic studies of Zeeman anticrossings in the \tilde{A}^1A_u state of the	(
acetylene molecule (C ₂ H ₂), P. Dupré, P.G. Green and R.W. Field	196 (1995) 211
Energy partitioning in photodissociation of methyl, ethyl and n-propyl iodides at 304 nm,	
W.K. Kang, K.W. Jung, D.C. Kim, KH. Jung and HS. Im	196 (1995) 363
Mass spectrometry	
Energy partitioning in photodissociation of methyl, ethyl and n-propyl iodides at 304 nm,	
W.K. Kang, K.W. Jung, D.C. Kim, KH. Jung and HS. Im	196 (1995) 363

Objects

Bulk systems

Dähne, A. Horvath and G. Weiser

•	
Gases	
Dissociation of acetyl bromide: an experimental and theoretical study, Y. Su, T.S. Dibble,	
J.S. Francisco and Z. Li	196 (1995) 59
Exchange-Coulomb potential energy surfaces, and related physical properties, for Kr-N2,	
A.K. Dham and W.J. Meath	196 (1995) 125
Transfer of vibrational energy to electronic excited states and vibration enhanced carbon	
production in optically excited V-V pumped CO, H.L. Wallaart, B. Piar, MY. Perrin	
and JP. Martin	196 (1995) 149
Quantum beat spectroscopic studies of Zeeman anticrossings in the \tilde{A}^1A_u state of the	
acetylene molecule (C ₂ H ₂), P. Dupré, P.G. Green and R.W. Field	196 (1995) 211
Study of Zeeman anticrossing spectra of the \tilde{A}^1A_u state of the acetylene molecule (C_2H_2)	
by Fourier transform: product $ ho_{ m vib}\langle V angle$ and isomerization barrier, P. Dupré	196 (1995) 239
Supersonic beams	
Metastable decay of ionic argon clusters: rotational predissociation of (Ar) ₄ ⁺ , E. Buonomo	
and F.A. Gianturco	196 (1995) 465
Liquid mixtures and solutions	
Far infrared interaction induced absorption spectra of CS2-C6H6 liquid mixtures. A low	
concentration study, E. Zoidis and T. Dorfmüller	196 (1995) 171
An infrared study of the interaction-induced vibrational spectra of benzene in liquid binary	
mixtures containing CS ₂ and C ₆ F ₆ , E. Zoidis, M. Besnard and J. Yarwood	196 (1995) 521
Excited-state geometries derived from the analysis of resonance Raman spectra. Example:	
$^{1}(\pi-\pi^{*})$ state of 3,5-di-tert-butyl-o-benzoquinone, H. Bettermann and I. Dasting	196 (1995) 531
Isomerisation dynamics of a thiacarbocyanine dye in different electronic states and in	
different classes of solvents, E. Vauthey	196 (1995) 569
Crystals	
Influence of aggregation on the optical spectra of a polymethine dye in single crystals, L.	
	(

NMR study of the $F-H\cdots F$ hydrogen bond. Relation between hydrogen atom position and $F-H\cdots F$ bond length, A.M. Panich	196 (1995) 511
Glasses	
Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na ₂ O-12.8CaO-50P ₂ O ₅ , V.M. Syutkin, V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina Diffusion of molecular oxygen in glassy matrices, studied by luminescence quenching, V.V. Korolev, V.V. Bolotsky, N.V. Shokhirev, E.B. Krissinel', V.A. Bagryansky and	196 (1995) 139
N.M. Bazhin	196 (1995) 317
Polymers	
On electron localization in periodic $(C_2H_nCl_{4-n})_x$ polymers, M. Springborg	196 (1995) 101
Plasmas	
Angular momentum state mixing and quenching of $n = 3$ atomic hydrogen fluorescence,	
B.L. Preppernau, K. Pearce, A. Tserepi, E. Wurzberg and T.A. Miller	196 (1995) 371
Catalytic properties of surfaces with respect to generation of CO ₂ molecules in the plasma, D.K. Otorbaev	106 (1005) 542
D.K. Otoroaev	196 (1995) 543
Microscopic systems	
Atoms	
The use of UV photoelectron spectroscopy to monitor production of excited states of atomic lead from the $Pb(^3P_0) + O_2(a^1\Delta_g)$ reaction, D. Haggerston, J.M. Dyke and A.	
Morris	196 (1995) 353
Angular momentum state mixing and quenching of $n = 3$ atomic hydrogen fluorescence, B.L. Preppernau, K. Pearce, A. Tserepi, E. Wurzberg and T.A. Miller	196 (1995) 371
Incipient manifestation of the shell structure of atoms within the WDA model for the exchange and kinetic energy density functionals, M.D. Glossman, L.C. Balbás and J.A.	
Alonso	196 (1995) 455
Molecules (neutral and ionic)	
-diatomic	
Pseudopotential calculations for the potential energies of LiHe and BaHe, E. Czuchaj, F. Rebentrost, H. Stoll and H. Preuss	196 (1995) 37
Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation	190 (1993) 37
of hydrogen fluoride, M. Sugawara and Y. Fujimura	196 (1995) 113
Photochemical population of KHg * states, D. Azinović, S. Milošević and G. Pichler	196 (1995) 267
Diffusion of molecular oxygen in glassy matrices, studied by luminescence quenching, V.V. Korolev, V.V. Bolotsky, N.V. Shokhirev, E.B. Krissinel', V.A. Bagryansky and	
N.M. Bazhin	196 (1995) 317
Spin-orbit configuration interaction study of the electronic spectrum of antimony iodide,	
K.K. Das, A.B. Alekseyev, HP. Liebermann, G. Hirsch and R.J. Buenker Dynamics of vibrationally inelastic collisions in H ⁺ -H ₂ : comparing quantum calculations	196 (1995) 395
with experiments, F.A. Gianturco and S. Kumar	196 (1995) 485

-small polyatomics	
A theoretical study on the structure of acetonitrile (CH ₃ CN) and its anion CH ₃ CN ⁻ , G.L.	
Gutsev, A.L. Sobolewski and L. Adamowicz	196 (1995) 1
Valence electron momentum distributions of ethylene; comparison of EMS measurements	
with near Hartree-Fock limit, configuration interaction and density functional theory	
calculations, B.P. Hollebone, J.J. Neville, Y. Zheng, C.E. Brion, Y. Wang and E.R.	
Davidson	196 (1995) 13
IR spectrum of HCF ₂ CF ₂ Br: hindered intramolecular vibrational energy redistribution, W.	190 (1993) 13
Fuß, K.L. Kompa and S. Weizbauer	196 (1995) 179
Quantum beat spectroscopic studies of Zeeman anticrossings in the \tilde{A}^1A_n state of the	190 (1993) 179
acetylene molecule (C_2H_2) , P. Dupré, P.G. Green and R.W. Field	106 (1005) 211
Study of Zeeman anticrossing spectra of the \tilde{A}^1A_u state of the acetylene molecule (C_2H_2)	196 (1995) 211
Study of Zeeman anticrossing spectra of the A A_u state of the acetylene molecule (C_2H_2)	10((1005) 220
by Fourier transform: product $\rho_{\text{vib}}(V)$ and isomerization barrier, P. Dupré	196 (1995) 239
Investigation of the predissociation of SO ₂ : state selective detection of the SO and O	104 (1005) 255
fragments, S. Becker, C. Braatz, J. Lindner and E. Tiemann	196 (1995) 275
Absolute oscillator strengths for the photoabsorption of silane in the valence and Si 2p and	
2s regions (7.5-350 eV), G. Cooper, G.R. Burton, W.F. Chan and C.E. Brion	196 (1995) 293
Energy partitioning in photodissociation of methyl, ethyl and <i>n</i> -propyl iodides at 304 nm,	
W.K. Kang, K.W. Jung, D.C. Kim, KH. Jung and HS. Im	196 (1995) 363
A theoretical analysis of the lowest excited states in HNO/NOH and HPO/POH, A. Luna,	
M. Merchán and B.O. Roos	196 (1995) 437
Broken dynamical symmetry condition to control a chemical reaction by the complex	
coordinate (t, t') method, O.E. Alon and N. Moiseyev	196 (1995) 499
An infrared study of the interaction-induced vibrational spectra of benzene in liquid binary	
mixtures containing CS ₂ and C ₆ F ₆ , E. Zoidis, M. Besnard and J. Yarwood	196 (1995) 521
Excited-state geometries derived from the analysis of resonance Raman spectra. Example:	
$(\pi - \pi^*)$ state of 3,5-di-tert-butyl-o-benzoquinone, H. Bettermann and I. Dasting	196 (1995) 531
An experimental and theoretical study of the valence shell photoelectron spectrum of	
allene, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A.	
MacDonald and W. von Niessen	196 (1995) 551
-aromatics	
Near-edge core photoabsorption in polyacenes: model molecules for graphite, H. Ågren, O.	
Vahtras and V. Carravetta	196 (1995) 47
Evidence for molecular distortion involving the carbonyl group in triplet states of carbonyl	(,
derivatives of naphthalene obtained from time resolved vibrational spectroscopic studies,	
M.J. van der Burgt, A.H. Huizer, C.A.G.O. Varma, B.D. Wagner and J. Lusztyk	196 (1995) 193
Single vibronic level fluorescence spectra from \tilde{A} ($^{1}B_{2u}$) benzene: Fermi resonances and S_{0}	170 (1770) 170
IVR lifetimes, J.A. Nicholson, W.D. Lawrance and G. Fischer	196 (1995) 327
An infrared study of the interaction-induced vibrational spectra of benzene in liquid binary	170 (1775) 527
mixtures containing CS ₂ and C ₆ F ₆ , E. Zoidis, M. Besnard and J. Yarwood	196 (1995) 521
mixtures containing CS ₂ and C ₆ r ₆ , L. Zoidis, M. Besnard and J. Talwood	190 (1993) 321
-other large	
Dissociation of acetyl bromide: an experimental and theoretical study, Y. Su, T.S. Dibble,	
J.S. Francisco and Z. Li	196 (1995) 59
v.o. Trancisco and L. Li	190 (1993) 39

Role of internal conversion on the excited state properties of trans-styrylpyridines, G. Marconi, G. Bartocci, U. Mazzucato, A. Spalletti, F. Abbate, L. Angeloni and E. Castellucci	196 (1995) 383
Isomerisation dynamics of a thiacarbocyanine dye in different electronic states and in	
different classes of solvents, E. Vauthey	196 (1995) 569
Molecular aggregates	
-dimers	
Representations of dispersion energy damping functions for interactions of closed shell atoms and molecules, A.K. Dham, A.R. Allnatt, A. Koide and W.J. Meath	196 (1995) 81
-van der Waals molecules	
Representations of dispersion energy damping functions for interactions of closed shell	
atoms and molecules, A.K. Dham, A.R. Allnatt, A. Koide and W.J. Meath	196 (1995) 81
Exchange-Coulomb potential energy surfaces, and related physical properties, for Kr-N ₂ ,	106 (1005) 125
A.K. Dham and W.J. Meath	196 (1995) 125
-clusters	
Far infrared interaction induced absorption spectra of CS_2 - C_6H_6 liquid mixtures. A low	
concentration study, E. Zoidis and T. Dorfmüller	196 (1995) 171
Metastable decay of ionic argon clusters: rotational predissociation of $(Ar)_4^+$, E. Buonomo and F.A. Gianturco	196 (1995) 465
-complexes	
Far infrared interaction induced absorption spectra of CS_2 - C_6H_6 liquid mixtures. A low	
concentration study, E. Zoidis and T. Dorfmüller	196 (1995) 171
Free radicals (including hydronium and muonium)	
Local description of a polyenic radical cation, P. Karafiloglou and G. Kapsomenos	196 (1995) 69
Catalytic properties of surfaces with respect to generation of CO ₂ molecules in the plasma,	
D.K. Otorbaev	196 (1995) 543
Quasiparticles (including excitons)	
Influence of aggregation on the optical spectra of a polymethine dye in single crystals, L.	
Dähne, A. Horvath and G. Weiser	196 (1995) 307
Ions and charge carriers	
Local description of a polyenic radical cation, P. Karafiloglou and G. Kapsomenos	196 (1995) 69
Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na ₂ O-12.8CaO-	
50P2O5, V.M. Syutkin, V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina	196 (1995) 139
Metastable decay of ionic argon clusters: rotational predissociation of (Ar) ₄ ⁺ , E. Buonomo	404 (4005)
and F.A. Gianturco	196 (1995) 465
Dynamics of vibrationally inelastic collisions in H ⁺ -H ₂ : comparing quantum calculations with experiments, F.A. Gianturco and S. Kumar	196 (1995) 485
with experiments, i.m. Giantareo and S. Kumai	190 (1993) 403

Phenomena

Molecular structure	
A theoretical study on the structure of acetonitrile (CH ₃ CN) and its anion CH ₃ CN Gutsev, A.L. Sobolewski and L. Adamowicz	-, G.L. 196 (1995) 1
Evidence for molecular distortion involving the carbonyl group in triplet states of c derivatives of naphthalene obtained from time resolved vibrational spectroscopic	arbonyl
M.J. van der Burgt, A.H. Huizer, C.A.G.O. Varma, B.D. Wagner and J. Lusztyl Single vibronic level fluorescence spectra from \tilde{A} (${}^{1}B_{2u}$) benzene: Fermi resonances	
IVR lifetimes, J.A. Nicholson, W.D. Lawrance and G. Fischer	196 (1995) 327
Electronic structure of donor–spacer–acceptor molecules of potential interest for molecules. III. Geometry and absorption spectrum of CH ₃ -α P3CNQ, A. Broo and Table 2012.	nd M.C.
Zerner Electronic structure of donor-spacer-acceptor molecules of potential interest for molecules	196 (1995) 407
electronics. IV. Geometry and device properties of P3CNQ and Q3CNQ, A. B	
M.C. Zerner	196 (1995) 423
A theoretical analysis of the lowest excited states in HNO/NOH and HPO/POH, A	
M. Merchán and B.O. Roos NMR study of the F-H · · · F hydrogen bond. Relation between hydrogen atom	196 (1995) 437
and F-H · · · F bond length, A.M. Panich	196 (1995) 511
Vibrations and rotations of molecules	
Evidence for molecular distortion involving the carbonyl group in triplet states of c derivatives of naphthalene obtained from time resolved vibrational spectroscopic	studies,
M.J. van der Burgt, A.H. Huizer, C.A.G.O. Varma, B.D. Wagner and J. Luszty	
Single vibronic level fluorescence spectra from \tilde{A} ($^{1}B_{2u}$) benzene: Fermi resonance: IVR lifetimes, J.A. Nicholson, W.D. Lawrance and G. Fischer	196 (1995) 327
Dynamics of vibrationally inelastic collisions in H ⁺ -H ₂ : comparing quantum calc	
with experiments, F.A. Gianturco and S. Kumar	196 (1995) 485
An infrared study of the interaction-induced vibrational spectra of benzene in liquid	
mixtures containing CS ₂ and C ₆ F ₆ , E. Zoidis, M. Besnard and J. Yarwood	196 (1995) 521
Electronic structure and states	
Valence electron momentum distributions of ethylene; comparison of EMS measure with near Hartree-Fock limit, configuration interaction and density functional calculations, B.P. Hollebone, J.J. Neville, Y. Zheng, C.E. Brion, Y. Wang a	l theory
Davidson	196 (1995) 13
Pseudopotential calculations for the potential energies of LiHe and BaHe, E. Czu	
Rebentrost, H. Stoll and H. Preuss	196 (1995) 37
Local description of a polyenic radical cation, P. Karafiloglou and G. Kapsomenos	s 196 (1995) 69 196 (1995) 101
On electron localization in periodic $(C_2H_nCl_{4-n})_x$ polymers, M. Springborg Absolute oscillator strengths for the photoabsorption of silane in the valence and S	
2s regions (7.5–350 eV), G. Cooper, G.R. Burton, W.F. Chan and C.E. Brion	196 (1995) 293
Influence of aggregation on the optical spectra of a polymethine dye in single cry	
Dähne, A. Horvath and G. Weiser	196 (1995) 307

Electronic structure of donor-spacer-acceptor molecules of potential interest for molecule electronics. III. Geometry and absorption spectrum of CH ₃ -α P3CNQ, A. Broo and M.G.	
Zerner	196 (1995) 407
Electronic structure of donor-spacer-acceptor molecules of potential interest for molecule electronics. IV. Geometry and device properties of P3CNQ and Q3CNQ, A. Broo are	nd
M.C. Zerner	196 (1995) 423
A theoretical analysis of the lowest excited states in HNO/NOH and HPO/POH, A. Lun M. Merchán and B.O. Roos	196 (1995) 437
Incipient manifestation of the shell structure of atoms within the WDA model for the exchange and kinetic energy density functionals, M.D. Glossman, L.C. Balbás and J.A.	Α.
Alonso	196 (1995) 455
Excited-state geometries derived from the analysis of resonance Raman spectra. Exampl ${}^{1}(\pi-\pi^{*})$ state of 3,5-di-tert-butyl-o-benzoquinone, H. Bettermann and I. Dasting	196 (1995) 531
An experimental and theoretical study of the valence shell photoelectron spectrum allene, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.	
MacDonald and W. von Niessen	196 (1995) 551
Spin splittings	
Spin-orbit configuration interaction study of the electronic spectrum of antimony iodic	le,
K.K. Das, A.B. Alekseyev, HP. Liebermann, G. Hirsch and R.J. Buenker	196 (1995) 395
Molecular interactions	
Representations of dispersion energy damping functions for interactions of closed she	ell
atoms and molecules, A.K. Dham, A.R. Allnatt, A. Koide and W.J. Meath	196 (1995) 81
Exchange-Coulomb potential energy surfaces, and related physical properties, for Kr-N	
A.K. Dham and W.J. Meath	196 (1995) 125
Far infrared interaction induced absorption spectra of CS ₂ -C ₆ H ₆ liquid mixtures. A lo	
concentration study, E. Zoidis and T. Dorfmüller	196 (1995) 171
Angular momentum state mixing and quenching of $n = 3$ atomic hydrogen fluorescene	
B.L. Preppernau, K. Pearce, A. Tserepi, E. Wurzberg and T.A. Miller	196 (1995) 371
Spectral bandshapes and intensities	
Pseudopotential calculations for the potential energies of LiHe and BaHe, E. Czuchaj,	F.
Rebentrost, H. Stoll and H. Preuss	196 (1995) 37
IR spectrum of HCF ₂ CF ₂ Br: hindered intramolecular vibrational energy redistribution,	W.
Fuß, K.L. Kompa and S. Weizbauer	196 (1995) 179
Absolute oscillator strengths for the photoabsorption of silane in the valence and Si 2p a	
2s regions (7.5-350 eV), G. Cooper, G.R. Burton, W.F. Chan and C.E. Brion	196 (1995) 293
Spin-orbit configuration interaction study of the electronic spectrum of antimony iodio K.K. Das, A.B. Alekseyev, HP. Liebermann, G. Hirsch and R.J. Buenker	de, 196 (1995) 395
Coupling of electronic and muslear motion	
Coupling of electronic and nuclear motion Pseudopotential calculations for the potential energies of LiHe and BaHe, E. Czuchaj,	F
Rebentrost, H. Stoll and H. Preuss	196 (1995) 37

Energy transfer processes	
Transfer of vibrational energy to electronic excited states and vibration enhanced carbon	
production in optically excited V-V pumped CO, H.L. Wallaart, B. Piar, MY. Perrin	
and JP. Martin	196 (1995) 149
Quantum beat spectroscopic studies of Zeeman anticrossings in the \tilde{A}^1A_u state of the	
acetylene molecule (C ₂ H ₂), P. Dupré, P.G. Green and R.W. Field	196 (1995) 211
Study of Zeeman anticrossing spectra of the \tilde{A}^1A_u state of the acetylene molecule (C_2H_2)	
by Fourier transform: product $ ho_{ m vib}\langle V angle$ and isomerization barrier, P. Dupré	196 (1995) 239
The use of UV photoelectron spectroscopy to monitor production of excited states of	
atomic lead from the $Pb(^{3}P_{0}) + O_{2}(a^{1}\Delta_{g})$ reaction, D. Haggerston, J.M. Dyke and A.	
Morris	196 (1995) 353
Molecular photophysical processes	
Near-edge core photoabsorption in polyacenes: model molecules for graphite, H. Ågren, O.	
Vahtras and V. Carravetta	196 (1995) 47
Dissociation of acetyl bromide: an experimental and theoretical study, Y. Su, T.S. Dibble,	
J.S. Francisco and Z. Li	196 (1995) 59
Photochemical population of KHg * states, D. Azinović, S. Milošević and G. Pichler	196 (1995) 267
Electronic structure of donor-spacer-acceptor molecules of potential interest for molecular	
electronics. IV. Geometry and device properties of P3CNQ and Q3CNQ, A. Broo and	
M.C. Zerner	196 (1995) 423
An experimental and theoretical study of the valence shell photoelectron spectrum of	
allene, P. Baltzer, B. Wannberg, M. Lundqvist, L. Karlsson, D.M.P. Holland, M.A.	105 (1005) 551
MacDonald and W. von Niessen	196 (1995) 551
Intramolecular dynamics	
IR spectrum of HCF ₂ CF ₂ Br: hindered intramolecular vibrational energy redistribution, W.	
Fuß, K.L. Kompa and S. Weizbauer	196 (1995) 179
Quantum beat spectroscopic studies of Zeeman anticrossings in the A A u state of the	
acetylene molecule (C ₂ H ₂), P. Dupré, P.G. Green and R.W. Field	196 (1995) 211
Study of Zeeman anticrossing spectra of the \tilde{A}^1A_u state of the acetylene molecule (C_2H_2)	
by Fourier transform: product $ ho_{ m vib}\langle V angle$ and isomerization barrier, P. Dupré	196 (1995) 239
Control of the yield of photophysical/photochemical processes by excitation with properly	
delayed ultrashort phase-locked light pulses: a model study on the pyrazine $S_2 \rightarrow S_1$	105 (1005) 115
internal conversion, A. Ferretti, A. Lami and G. Villani	196 (1995) 447
Metastable decay of ionic argon clusters: rotational predissociation of (Ar) ₄ ⁺ , E. Buonomo	106 (1005) 465
and F.A. Gianturco Broken dynamical symmetry condition to control a chemical reaction by the complex	196 (1995) 465
coordinate (t, t') method, O.E. Alon and N. Moiseyev	196 (1995) 499
cooldinate (1, 1) method, O.E. Alon and W. Moiseyev	190 (1993) 499
-radiationless transitions	
Role of internal conversion on the excited state properties of trans-styrylpyridines, G.	
Marconi, G. Bartocci, U. Mazzucato, A. Spalletti, F. Abbate, L. Angeloni and E.	
Castellucci	196 (1995) 383
Control of the yield of photophysical/photochemical processes by excitation with properly	
delayed ultrashort phase-locked light pulses: a model study on the pyrazine $S_2 \rightarrow S_1$	106 (1005) 447
internal conversion, A. Ferretti, A. Lami and G. Villani	196 (1995) 447

Isomerisation dynamics of a thiacarbocyanine dye in different electronic states and in different classes of solvents, E. Vauthey	196 (1995) 569
 -vibrational energy redistribution (including vibrational dissociation) Transfer of vibrational energy to electronic excited states and vibration enhanced carbon production in optically excited V-V pumped CO, H.L. Wallaart, B. Piar, MY. Perrin and JP. Martin IR spectrum of HCF₂CF₂Br: hindered intramolecular vibrational energy redistribution, W. Fuß, K.L. Kompa and S. Weizbauer 	196 (1995) 149 196 (1995) 179
Luminescence spectra, yields and lifetimes Role of internal conversion on the excited state properties of trans-styrylpyridines, G. Marconi, G. Bartocci, U. Mazzucato, A. Spalletti, F. Abbate, L. Angeloni and E. Castellucci	196 (1995) 383
Multiphoton phenomena Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation of hydrogen fluoride, M. Sugawara and Y. Fujimura	196 (1995) 113
Reactions (including dissociation) Catalytic properties of surfaces with respect to generation of ${\rm CO_2}$ molecules in the plasma, D.K. Otorbaev	196 (1995) 543
-gas phase Control of quantum dynamics by a locally optimized laser field. Multi-photon dissociation of hydrogen fluoride, M. Sugawara and Y. Fujimura Photochemical population of KHg * states, D. Azinović, S. Milošević and G. Pichler The use of UV photoelectron spectroscopy to monitor production of excited states of atomic lead from the Pb(³ P ₀) + O ₂ (a ¹ Δ _g) reaction, D. Haggerston, J.M. Dyke and A. Morris Catalytic properties of surfaces with respect to generation of CO ₂ molecules in the plasma,	196 (1995) 113 196 (1995) 267 196 (1995) 353
D.K. Otorbaev -condensed phase	196 (1995) 543
Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na ₂ O-12.8CaO-50P ₂ O ₅ , V.M. Syutkin, V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina Isomerisation dynamics of a thiacarbocyanine dye in different electronic states and in different classes of solvents, E. Vauthey	196 (1995) 139 196 (1995) 569
 -photochemical Investigation of the predissociation of SO₂: state selective detection of the SO and O fragments, S. Becker, C. Braatz, J. Lindner and E. Tiemann Energy partitioning in photodissociation of methyl, ethyl and n-propyl iodides at 304 nm, 	196 (1995) 275
W.K. Kang, K.W. Jung, D.C. Kim, KH. Jung and HS. Im Role of internal conversion on the excited state properties of trans-styrylpyridines, G. Marconi, G. Bartocci, U. Mazzucato, A. Spalletti, F. Abbate, L. Angeloni and E. Castellucci	196 (1995) 363 196 (1995) 383

Broken dynamical symmetry condition to control a chemical reaction by the complex coordinate (t, t') method, O.E. Alon and N. Moiseyev	196 (1995) 499
Electron transfer	
Local description of a polyenic radical cation, P. Karafiloglou and G. Kapsomenos	196 (1995) 69
Electronic structure of donor-spacer-acceptor molecules of potential interest for molecular electronics. IV. Geometry and device properties of P3CNQ and Q3CNQ, A. Broo and	
M.C. Zerner	196 (1995) 423
Dynamics of vibrationally inelastic collisions in H ⁺ -H ₂ : comparing quantum calculations	
with experiments, F.A. Gianturco and S. Kumar	196 (1995) 485
Ionization (including Rydberg states)	
Absolute oscillator strengths for the photoabsorption of silane in the valence and Si 2p and	
2s regions (7.5-350 eV), G. Cooper, G.R. Burton, W.F. Chan and C.E. Brion	196 (1995) 293
Molecular motion (including diffusive)	
Diffusion of silver ions towards radiation-induced traps in the glass 37.2Na ₂ O-12.8CaO-	
50P ₂ O ₅ , V.M. Syutkin, V.A. Tolkatchev, A.V. Dmitryuk and S.E. Paramzina	196 (1995) 139
Diffusion of molecular oxygen in glassy matrices, studied by luminescence quenching,	
V.V. Korolev, V.V. Bolotsky, N.V. Shokhirev, E.B. Krissinel', V.A. Bagryansky and	
N.M. Bazhin	196 (1995) 317
Thermodynamic and transport properties	
Exchange-Coulomb potential energy surfaces, and related physical properties, for Kr-N ₂ ,	
A.K. Dham and W.J. Meath	196 (1995) 125
Structure of solids and liquids	
NMR study of the F-H · · · F hydrogen bond. Relation between hydrogen atom position	
and F-H · · · F bond length, A.M. Panich	196 (1995) 511